

Universality of Fragmentation in the Schrödinger Dynamics of Bosonic Josephson Junctions

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Abstract

The many-body Schrödinger dynamics of a one-dimensional bosonic Josephson junction is investigated for up to ten thousand bosons and long times. The initial states are fully condensed and the interaction strength is weak. We report on a universal fragmentation dynamics on the many-body level: systems consisting of different numbers of particles fragment to the same value at constant mean-field interaction strength. Using the Bose-Hubbard model we show how the value of the universal fragmentation dynamics can be predicted from the initial state. The analysis allows the prediction of the extent to which many-body effects become important in the dynamics at much later times. Even for the largest particle numbers and the weakest interaction strengths the dynamics is many-body in nature and the fragmentation universal. Implications are discussed.

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Over the last few years ultracold bosons in double-well potentials have made it possible to explore quantum many-body dynamics in a highly controllable manner. Among the phenomena predicted or observed are tunneling and self-trapping [1–5], Josephson oscillations [2–5], collapse and revival sequences [1], squeezing [6], matter wave interferometry [7], fragmentation and the approach to an equilibrium state [8–12]. While tunneling, self-trapping and Josephson oscillations have explanations on the mean-field level, other phenomena, e.g., collapse and revival sequences require many-body treatments such as the Bose-Hubbard model [1] or even the full many-body Schrödinger equation [12, 13].

In the context of bosonic Josephson junctions self-trapping – the inhibition of tunneling due to interparticle interactions – is a theoretically and experimentally well-studied phenomenon [1–4]. Within two-mode Gross-Pitaevskii (GP) mean-field theory an explicit criterion was derived that determines whether self-trapping occurs for a given condensed initial state or not [1, 2]. The mean-field theory reduces the many-body quantum dynamics to that of a classical nonrigid pendulum and self-trapping occurs from a critical value of the interaction strength onwards [1, 2]. The theory was successfully applied in the description of experiments at short time scales [3–5]. However, for longer times the dynamics can leave the realm of mean-field theory and make a many-body description necessary, especially when the number of bosons is in the hundreds and the interaction strength is strong enough for self-trapping to occur, see, e.g., Refs. [1, 12, 14, 15].

Here, we investigate the long-time many-body dynamics of Bose-Einstein condensates (BECs) forming bosonic Josephson junctions with up to ten thousand bosons in the condensate. We consider interactions that are so weak that self-trapping *cannot* occur. The BECs are initially fully condensed. We then solve the time-dependent many-body Schrödinger equation for these BECs numerically. This letter contains the following main results. Firstly, we report on the existence of a *universal* many-body fragmentation dynamics in bosonic Josephson junctions. Fragmentation is a basic many-boson phenomenon which is – usually – strongly dependent on the number of bosons in the system [8–12]. Here we find that systems consisting of different numbers of bosons all fragment to the same value at fixed mean-field interaction strength. The appearance of such universal fragmentation dynamics on the many-body level is unexpected. Moreover, this dynamical fragmentation implies the breakdown of GP mean-field theory. Above the critical interaction strength for self-trapping mean-field theory is known to break down on a time scale that increases logarithmically

with the number of particles [15]. Here, we find such a logarithmic breakdown even below the critical interaction strength.

Secondly, using the Bose-Hubbard (BH) model we show how the universal fragmentation dynamics is related to the initial conditions. For a whole class of condensed initial states our analysis makes it possible to predict the fragmentation of the BEC after the collapse of the density oscillations, and thus to predict the extent to which the many-body dynamics for these condensed initial states remains within the realm of mean-field theory. Thirdly, we show that even for extremely weak interactions the dynamics remains many-body in nature, indicating that there is no limit at which GP theory becomes valid at long times. The results allow the extrapolation to larger particle numbers.

In order to compute the time-evolution of the many-body Schrödinger equation we use the MultiConfigurational Time-Dependent Hartree for Bosons (MCTDHB) method [16], see also Refs. [12, 13, 17, 18]. It is convenient to use dimensionless units defined by dividing the Hamiltonian by $\frac{\hbar^2}{mL^2}$, where m is the mass of a boson and L is a length scale. The full many-body Hamiltonian then reads

$$H = \sum_{i=1}^N h(x_i) + \sum_{i<j} W(x_i - x_j), \quad (1)$$

where $h(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)$ with a trapping potential $V(x)$ and an interparticle interaction potential $W(x-x') = \lambda_0\delta(x-x')$. For the potential $V(x)$ we choose a double-well constructed by connecting two harmonic potentials $V_{\pm}(x) = \frac{1}{2}(x \pm 2)^2$ with a natural cubic spline at $|x| = 0.5$. Using the left- and right-localized orbitals $\phi_{L,R}$ constructed from the ground and first excited state of $V(x)$ the parameters $J \equiv -\langle\phi_L|h|\phi_R\rangle = 2.2334 \times 10^{-2}$, $U = \lambda_0 \int |\phi_L|^4$, $\Lambda = U(N-1)/(2J)$, and $t_{Rabi} = \pi/J = 140.66$ are computed.

All one-body observables can be computed from the first-order reduced density matrix $\rho^{(1)}(x|x') = \langle\Psi|\hat{\Psi}^\dagger(x')\hat{\Psi}(x)|\Psi\rangle = \sum_i n_i^{(1)}\alpha_i^{(1)}(x)\alpha_i^{(1)*}(x')$, where $\hat{\Psi}(x)$ denotes the bosonic field operator, $|\Psi\rangle$ the many-boson wavefunction, $\alpha_i^{(1)}(x)$ the natural orbitals, and $n_1^{(1)} \geq n_2^{(1)}, \dots$ the natural occupations with $\sum_i n_i^{(1)} = N$. We suppress the time-argument whenever unambiguous. Bose-Einstein condensation is defined as follows: if an eigenvalue $n_i^{(1)} = \mathcal{O}(N)$ exists, the system is condensed [19]. If there is more than one such eigenvalue, the BEC is said to be fragmented [8–10, 20, 21]. Here, it is convenient to define the fragmentation as $f \equiv \sum_{i>1} n_i^{(1)}/N$. In GP theory $f = 0\%$ at all times, by construction. On the many-body

Schrödinger level this need not be the case and $100\% > f \geq 0\%$. Fragmentation ($f > 0$) is accompanied by a loss of coherence [21].

We compute the many-body dynamics for condensed states which are the GP ground states of the potential $V_+(x)$. Thus, initially the BECs are located in the left well. For each particle number N we choose the interaction strength λ_0 such that $\lambda = \lambda_0(N - 1)$ is constant. The parameter λ appears in the GP equation and is known as the mean-field interaction strength. Increasing N at constant λ implies a decreasing interaction strength λ_0 . For the following computations we fix the mean-field interaction strength at $\lambda = 0.152$ which is equivalent to $\Lambda = 1.33$, i.e., well below the critical value $\Lambda_c = 2$ for self-trapping [1, 2].

Fig. 1 (top) shows the probability in the left well $p_L(t) = \frac{1}{N} \int_{-\infty}^0 \rho^{(1)}(x|x;t)dx$ as a function of time for $N = 100 - 10000$ bosons. The density tunnels back and forth through the potential barrier and eventually the density oscillations collapse. For larger N the collapse takes longer. The collapse occurs on the many-body level, but not within GP mean-field theory [1, 12]. We will therefore investigate the many-body nature of the BEC during the collapse in more detail. In Fig. 1 (bottom) the corresponding natural occupations are shown. Since the many-body wavefunction is initially condensed, there is only one natural occupation $n_1^{(1)} = N$ at $t = 0$. However, as time increases a second natural orbital becomes occupied and the system starts to fragment. The nature of the BEC changes from condensed to fragmented as the density oscillations collapse. We stress here that these results represent the many-body Schrödinger dynamics of the Hamiltonian (1) [22].

Looking at Fig. 1 we observe that the fragmentation dynamics is universal: at constant λ systems consisting of *different* numbers of bosons fragment to the *same* value during the collapse of the density oscillations. At the end of the collapse the two largest natural occupations reach plateaus at about $n_1^{(1)}/N = 66\%$ and $n_2^{(1)}/N = 34\%$. Thus, the fragmentation after the initial collapse of the density oscillations, f_{col} , settles at a value of $f_{col} = 34\%$, regardless of the number of particles involved. Note that the GP mean-field has universal dynamics firmly built into the theory; the GP dynamics is identical for all systems with the same value of λ . However, here we report on a universal fragmentation dynamics which is only present on the many-body level. Fragmentation is usually strongly dependent on the number of particles in the system [8–12]. Hence, the appearance of a universal fragmentation dynamics is unexpected.

Let us discuss the time scales involved in this universal fragmentation dynamics. We define the fragmentation time T_{frag} as the first time at which a certain fragmentation f is reached. Fig. 2 (top) shows the fragmentation time T_{frag} as a function of N . Clearly, T_{frag} increases with N . For any value of the fragmentation, T_{frag} is well described by a fit to the function $T(N) = a \ln(1 + bN)$, as is shown here for the values $f = 4\%, 9\%, \dots, 34\%$. Thus, T_{frag} grows logarithmically with N . Consequently, the fragmentation does not decrease or even disappear in the limit of large N . Even for $N = 10000$ bosons the fragmentation rises to about 10% in less than a dozen t_{Rabi} .

Since GP theory does not allow BECs to fragment at all, T_{frag} defines a measure for the breakdown of mean-field theory. It is well-known that mean-field theory can break down, especially for small particle numbers and on time scales of several t_{Rabi} , see, e.g., Refs. [1, 12, 14, 15]. In Ref. [15] it was shown that the time after which GP theory breaks down scales logarithmically with N for $\Lambda = 4$, way above the critical interaction strength for self-trapping $\Lambda_c = 2$. Here, we find that the fragmentation time T_{frag} scales logarithmically with N at $\Lambda = 1.33$, i.e., well below Λ_c . Hence, the logarithmic breakdown of mean-field theory cannot be attributed to a mean-field instability [15] and more research needs to be done to explain this scaling.

So far we have established the universality of fragmentation of the many-body Schrödinger dynamics and discussed some implications. We will now analyze this dynamics on the basis of a simple model and show that the universality of fragmentation is a general phenomenon that exists for a wide range of initial conditions and interaction strengths. As a model we use the two-mode BH Hamiltonian

$$\hat{H}_{BH} = -J \left(\hat{b}_L^\dagger \hat{b}_R + \hat{b}_R^\dagger \hat{b}_L \right) + \frac{U}{2} \left(\hat{b}_L^\dagger \hat{b}_L^\dagger \hat{b}_L \hat{b}_L + \hat{b}_R^\dagger \hat{b}_R^\dagger \hat{b}_R \hat{b}_R \right), \quad (2)$$

where the operators $b_{L,R}^\dagger$ create bosons in the orbitals $\phi_{L,R}$, respectively. The probability in the left well reads $p_L(t) = \frac{1}{N} \langle \hat{b}_L^\dagger \hat{b}_L \rangle(t)$ and the fragmentation of the BEC reduces here to the occupation of the second natural orbital, $f = n_2^{(1)}/N \leq 50\%$. We consider the family of condensed states given by

$$|\Psi_0\rangle = \frac{1}{\sqrt{N!}} \left(\sqrt{p_L(0)} \hat{b}_L^\dagger + \sqrt{p_R(0)} \hat{b}_R^\dagger \right)^N |0\rangle, \quad (3)$$

where $p_R(0) = 1 - p_L(0)$.

We choose parameter values corresponding to $\Lambda = 1.33$ and solve the dynamics of the Hamiltonian (2). We find that for the entire family of initial states $|\Psi_0\rangle$ with $0 \leq p_L(0) \leq 1$,

BECs consisting of different numbers of particles fragment to the same value f_{col} during the collapse of the density oscillations. Thus, also the BH fragmentation dynamics is universal. This can be seen in Fig. 3 (left) where the fragmentation f is shown as a function of time for $N = 1000$ and 10000 bosons. The fragmentation of initial states with $p_L(0) = 1.0$ reaches a plateau at about $f_{col} = 32\%$, not far from the many-body Schrödinger result 34% , see Fig. 1 (bottom). Similarly, initial states with $p_L(0) = 0.8$ fragment towards the value $f_{col} = 16\%$. Thus, the universal fragmentation dynamics is a general phenomenon which exists for a whole family of initially-condensed systems.

We will now point out a striking relation that allows the prediction of the value of f_{col} from the initial state. To this end we solve the BH eigenvalue problem $\hat{H}_{BH}|E_n\rangle = E_n|E_n\rangle$. Fig. 3 (right) shows the fragmentation f_n of each eigenstate $|E_n\rangle$ as a function of E_n/N . Note that the curves for the eigenstate fragmentation $f_n \equiv f_n(E_n/N)$ practically do not depend on the particle number, as shown here explicitly for $N = 1000$ and 10000 bosons. Also shown are the expansion coefficients $C_n = \langle E_n|\Psi_0\rangle$ of the initial states together with their energies per particle $E/N = \langle \Psi_0|\hat{H}_{BH}|\Psi_0\rangle/N$. As a function of E_n/N the coefficients are approximately binomially distributed with a width $\sim N^{-1/2}$. We find that for eigenstates with energy $E_n \approx E$ the eigenstate fragmentation equals the fragmentation of the many-body system after the collapse of the density oscillations, namely $f_n(E_n/N \approx E/N) = f_{col}$. This surprising empirical result links the condensed initial states (3) to the fragmentation of the many-body wavefunction after the collapse of the density oscillations, i.e., at much later times. We have checked this relation for up to $N = 10000$ bosons. However, the results shown in Fig. (3) suggest that an extrapolation to any number of bosons can be made. Based on these findings it is possible to predict to what extent the condensed initial states (3) will fragment during the collapse of the density oscillations. We note that fragmentation manifests itself in observables such as the fringe visibility and correlation functions which are experimentally accessible, see, e.g., Refs. [15, 21, 23].

Let us briefly touch upon the question whether fragmentation disappears for ever weaker interaction strength. Therefore, we choose an interaction strength which is only a tenth of the interaction strength considered so far, $\lambda = 0.0152$ ($\Lambda = 0.133$). The results are shown in Fig. 4. Again, the BECs fragment and the fragmentation dynamics is universal. Note that the time scale is much larger now. Initial states with $p_L(0) = 1.0$ now fragment to about $f_{col} = 48\%$ which is higher than for stronger interaction, initial states with $p_L(0) = 0.8$

to about $f_{col} = 10.5\%$ which is lower than for stronger interaction. These results are in agreement with the predictions of the here proposed model for universal fragmentation: we find again that $f_n(E_n/N \approx E/N) = f_{col}$. The results also show that the GP mean-field dynamics is not recovered despite the weaker interaction strength.

Summarizing, we have shown that there is a universal fragmentation dynamics in bosonic Josephson junctions at weak interaction strengths by solving the time-dependent many-boson Schrödinger equation. We have shown how the value of this universal fragmentation can be predicted from the initial state using the two-mode BH model. The GP mean-field dynamics is not recovered in the limit of large particle numbers, despite weak interaction strength.

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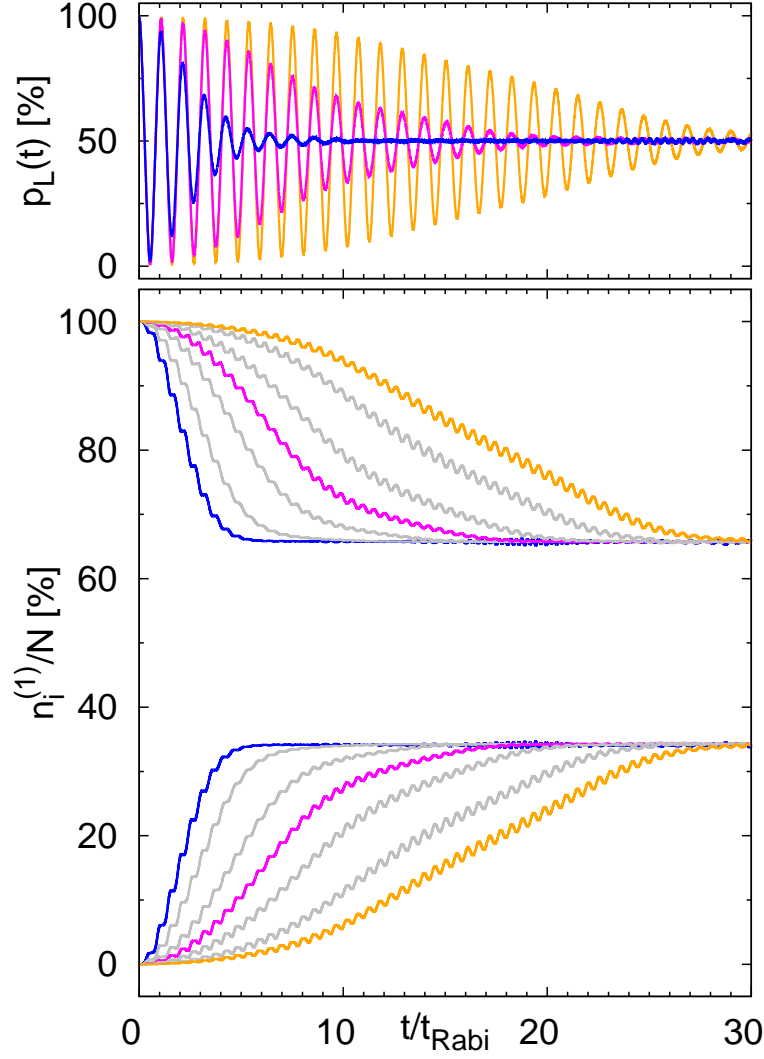


Figure 1. (color online): Universality of the many-body Schrödinger fragmentation dynamics. Shown is the probability in the left potential well $p_L(t)$ (top) and the corresponding natural occupations $n_i^{(1)}$ (bottom) as a function of time for different particle numbers. During the collapse of the density oscillations (top) the nature of the BEC changes from condensed to fragmented (bottom). The fragmentation reaches a plateau at $f_{col} = 34\%$ for all particle numbers. Interaction strength: $\lambda = 0.152$ ($\Lambda = 1.33$). Particle numbers: $N=100$ (blue), 1000 (magenta), 10000 (orange). The grey lines represent particle numbers in between, $N=200, 500, 2000$ and 5000 . All quantities shown are dimensionless.

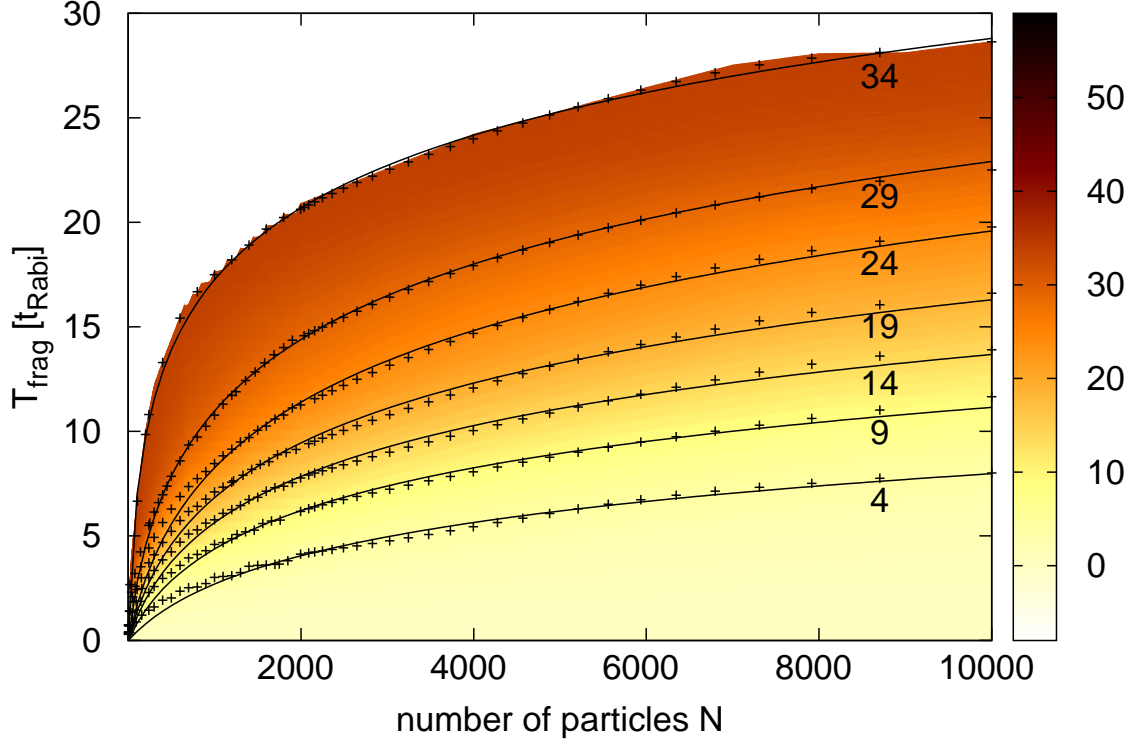


Figure 2. (color online): Fragmentation times. Shown are the times T_{frag} that are needed to reach a given fragmentation f as a function of the number of bosons for the same parameters as in Fig. 1. The data points (crosses) of all fragmentation values are well described by a logarithmic fit function (lines), here shown for the values $f = 4\%, 9\%, \dots, 34\%$. This logarithmic dependence of T_{frag} on the number of particles implies the breakdown of GP mean-field theory even in the limit of large particle numbers. Note that the logarithmic dependence occurs already at an interaction strength $\Lambda = 1.33$, well below the critical mean-field interaction strength $\Lambda_c = 2$. See text for details. All quantities shown are dimensionless.

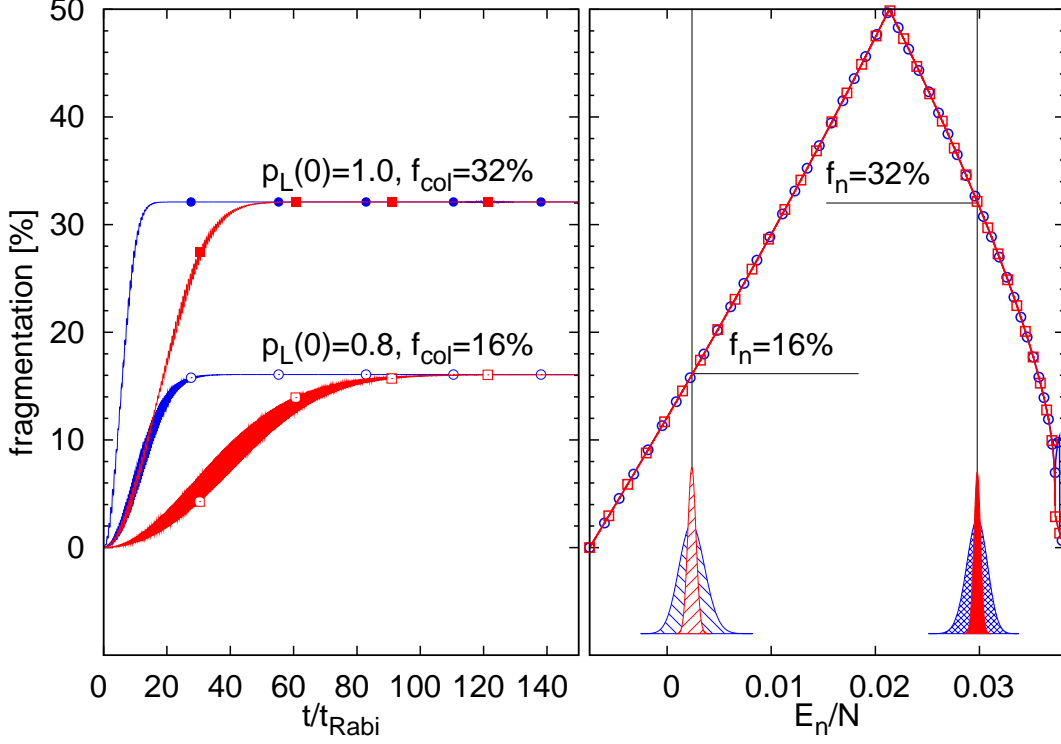


Figure 3. (color online): Universality of the BH fragmentation dynamics. Interaction strength $\lambda = 0.152$ ($\Lambda = 1.33$). Left: Shown is the fragmentation dynamics of fully condensed initial states with different numbers of particles in the left well $p_L(0)$. Parameter values: $N = 1000, p_L(0) = 1.0$: \bullet , $N = 1000, p_L(0) = 0.8$: \circ , $N = 10000, p_L(0) = 1.0$: \square , $N = 10000, p_L(0) = 0.8$: \blacksquare . The fragmentation reaches a plateau at about $f_{\text{col}} = 32\%$ ($f_{\text{col}} = 16\%$) for initial states with $p_L(0) = 1.0$ ($p_L(0) = 0.8$). Right: Shown is the fragmentation f_n of each eigenstate as a function of its energy per particle E_n/N for different particle numbers ($N=1000$: \circ , $N=10000$: \square). Also shown are the energies per particle of the initial states E/N (vertical lines) together with the distributions of the expansion coefficients C_n as shaded areas ($N=1000$: blue, $N=10000$: red). For eigenstates with $E_n \approx E$ the fragmentation of the many-boson wavefunction after the collapse is given by $f_{\text{col}} = f_n$ for any value of $p_L(0)$. All quantities shown are dimensionless.

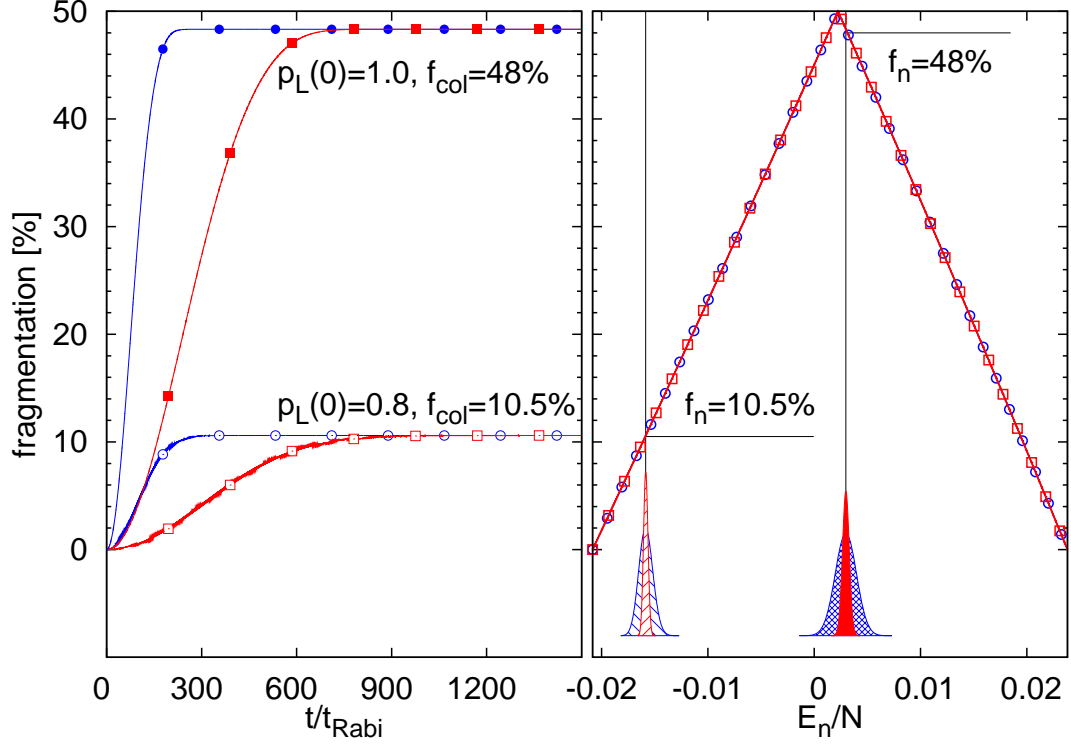


Figure 4. (color online): Same as in Fig. 3, but for ten times smaller interaction strength $\lambda = 0.0152$ ($\Lambda = 0.133$), far below the critical interaction strength $\Lambda_c = 2$. See text for more details. All quantities shown are dimensionless.